

$\text{Ce}_3[\text{PO}_4]\text{Cl}_6$ $hP32$ $(176) P6_3/m - h^4f^2$ **$\text{Ce}_3(\text{PO}_4)\text{Cl}_6$ [1]**

Structural features: $\text{Ce}(\text{Cl}_6\text{O}_2)(\text{ClO})$ bicapped square antiprisms share atoms to form a 3D-framework; P in tetrahedral voids (partial disorder). Variant of $\text{La}_3(\text{VO}_4)\text{Cl}_6$.

Sieke C., Schleid T. (2001) [1]

 $\text{Ce}_3\text{Cl}_6\text{O}_4\text{P}$

$a = 1.24636$, $c = 0.40693$ nm, $c/a = 0.326$, $V = 0.5474$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	$6h$	$m..$	0.1443	0.2557	$\frac{1}{4}$		non-colinear Ce_2 non-colinear O_2 trigonal bipyramid Ce_4O
O2	$6h$	$m..$	0.2252	0.5376	$\frac{1}{4}$		
Ce3	$6h$	$m..$	0.4187	0.28599	$\frac{1}{4}$		
Cl4	$6h$	$m..$	0.4411	0.0615	$\frac{1}{4}$		
P5	$4f$	$3..$	$\frac{1}{3}$	$\frac{2}{3}$	0.187	0.5	
O6	$4f$	$3..$	$\frac{1}{3}$	$\frac{2}{3}$	0.686	0.5	

Transformation from published data: $y, x, -z$; origin shift $0\ 0\ \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.028$

Remarks: Refinement of the occupancies of sites P5 and O6 showed no significant deviation from 0.5. Short interatomic distances for partly occupied site(s).

References: [1] Sieke C., Schleid T. (2001), Z. Anorg. Allg. Chem. 627, 761-767.